Spectral properties of reduced fermionic density operators and superselection rules

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Abstract

We consider pure fermionic states with varying number of quasiparticles and demonstrate that spectra of partial states (reduced with respect to some bipartition) are not identical as it takes place for bosons and conventional states in spaces with tensor product structure. We fully characterize pure states with equispectral partial states and show that they are related via local unitary operations with states satisfying the parity superselection rule [1]. Thus, valid purifications for fermionic density operators are found. As a byproduct, the positive semidefinite density matrix for fermions is constructed without implying the state gaussianity. The developed formalism clearly indicates that the conventional partial trace methods are not applicable to fermionic systems.

Notation

Consider the algebra of canonical anticommutation relations (CAR algebra) $\mathcal{A}$ generated by the ladder operators $a_k, a_k^\dagger$ satisfying the relations [2,3]

$$a_k a_s^\dagger + a_s^\dagger a_k = \delta_{ks} I,$$
$$a_k a_s + a_s a_k = a_k^\dagger a_s^\dagger + a_s^\dagger a_k^\dagger = 0,$$

where $k, s = 1, \ldots, n$. Let H_n be the Hilbert space with the dimension $\dim H_n = 2^n$ and $\{|j_1 \ldots j_n\rangle\}$ be the fixed orthonormal basis, where indices $j_s = 0, 1$. We shall suppose that $\mathcal{A}$ is realized as the algebra of all bounded operators in H_n such that

$$a_k^\dagger |j_1 \ldots j_n\rangle = \begin{cases} (-1)^{\sum_{s=1}^{k-1} j_s} |j_1 \ldots j_{k-1}\, 1\, j_{k+1} \ldots j_n\rangle, & j_k = 0, \\ 0, & j_k = 1, \end{cases}$$

and a_k is conjugate to $a_k^\dagger$.

Definition 1 *The state $|\psi\rangle$ satisfies the parity superselection rule if a unit vector $|\psi\rangle \in H$ has the form*

$$\psi = \sum_{j_1,\ldots,j_n \in \{0,1\}} \lambda_{j_1 \ldots j_n} |j_1 \ldots j_n\rangle, \quad \lambda_{j_1 \ldots j_n} \in \mathbb{C}, \qquad (1)$$

where all the numbers $\sum_k j_k$ are even or odd alternatively for all non-zero $\lambda_{j_1 \ldots j_n}$.

Definition 2 *The state ω is said to be even if*

$$\omega(a_{j_1}^\# \ldots a_{j_{2k+1}}^\#) = 0$$

for any choice of ladder operators $a_s^\# = a_s$ or $a_s^\dagger$, $s = 1, \ldots, 2k+1$.

Proposition 1 *The pure state ω is even iff it satisfies the parity superselection rule.*

Proof. Suppose that ω satisfies the parity superselection rule. Consider the representation (1). Since the odd order monomial $a_{j_1}^\# \ldots a_{j_{2k+1}}^\#$ changes even number of particles to the odd one and vice versa, the vectors $a_{j_1}^\# \ldots a_{j_{2k+1}}^\# |j_1 \ldots j_n\rangle$ corresponding to non-zero terms in (1) are pairwise orthogonal for any choice of $a_s^\#$. It follows that ω is even.
If ω does not satisfy the parity superselection rule, then its representation in the form of (1) contains at least two non-zero terms, say $|j_1 \ldots j_n\rangle$ and $|\tilde{j}_1 \ldots \tilde{j}_n\rangle$, such that $\sum_k j_k$ and $\sum_k \tilde{j}_k$ have different parity. There exists the unique monomial of odd order $a_{k_1} \ldots a_{k_{2s+1}}$, which is a partial isometrical operator mapping $|j_1 \ldots j_n\rangle$ to $|\tilde{j}_1 \ldots \tilde{j}_n\rangle$ and reset to zero all the other basis vectors. Thus, the value of ω does not equal zero on this monomial. Hence, ω can not be even. □

Reduced fermionic density matrices

Let $\mathcal{A}$ be obtained by joining two algebras of canonical anticommutation relations $\mathcal{A}_1$ and $\mathcal{A}_2$ with the generators $\{a_1, a_1^\dagger, \ldots, a_m, a_m^\dagger\}$ and $\{a_{m+1}, a_{m+1}^\dagger, \ldots, a_n, a_n^\dagger\}$, respectively. Fix a unit vector $|\psi\rangle \in H$.

Definition 3 *The states $\omega_j(x) = \langle\psi|x|\psi\rangle$, $x \in \mathcal{A}_j$ that are the restrictions of a pure state $|\psi\rangle\langle\psi|$ to the algebras $\mathcal{A}_j$, $j = 1, 2$, are said to be reduced (partial) states of $|\psi\rangle\langle\psi|$.*

Let us consider n fermionic modes and the corresponding CAR algebra $\mathcal{A}$, $\dim\mathcal{A} = 4^n$. The generators of $\mathcal{A}$ are $a_s a_s^\dagger$, a_s, $a_s^\dagger$, and $a_s^\dagger a_s$, $s = 1, \ldots, n$. Binary representation of numbers $0, \ldots, 2^n - 1$ forms the set of multiindices $\mathcal{J} \ni J = (j_1, \ldots, j_n)$, $j_s \in \{0, 1\}$. Given two multiindices $J, K \in \mathcal{J}$, let us define $A_{JK} \in \mathcal{A}$ by the formula

$$A_{JK} = c_{j_1}^\dagger c_{j_2}^\dagger \ldots c_{j_n}^\dagger c_{k_n} \ldots c_{k_2} c_{k_1}, \qquad (2)$$

where

$$c_{j_s}^\dagger = \begin{cases} a_s a_s^\dagger & \text{if } j_s = 0, \\ a_s^\dagger & \text{if } j_s = 1; \end{cases} \qquad c_{k_s} = \begin{cases} a_s a_s^\dagger & \text{if } k_s = 0, \\ a_s & \text{if } k_s = 1. \end{cases}$$

Proposition 2 *The following relation holds:*

$$A_{JK} = |j_1 \ldots j_n\rangle\langle k_1 \ldots k_n|.$$

Proof. Consider the operator $C_K = c_{k_n} \ldots c_{k_1}$, which is a rank one partial isometry in the sense that $C_K = |\varphi\rangle\langle\chi|$ for some unit vectors $|\varphi\rangle, |\chi\rangle \in H$ that are either orthogonal or coincide. Moreover, $C_K |k_1 \ldots k_n\rangle = |0 \ldots 0\rangle$. Then, $A_{JK} = C_J^\dagger C_K$. □

Corollary 1 *The element $\rho \in \mathcal{A}$ defines a valid quantum state iff it can be represented in the form*

$$\rho = \sum_{J,K \in \mathcal{J}} \lambda_{JK} A_{JK}, \qquad (3)$$

where (λ_{JK}) is a positive semidefinite matrix with the unit trace $\sum_J \lambda_{JJ} = 1$ (fermionic density matrix).

Corollary 2 *The $2^n \times 2^n$ matrix with elements $\langle A_{KJ}\rangle$ is a density matrix of an n-mode fermionic state over which the average is taken.*

Example. Using Eq. (2) and Corollary 2, the 2-mode fermionic state can be described by the density matrix

$$\begin{pmatrix} \langle a_1 a_1^\dagger a_2 a_2^\dagger\rangle & \langle a_1 a_1^\dagger a_2^\dagger\rangle & \langle a_1^\dagger a_2 a_2^\dagger\rangle & \langle a_1^\dagger a_2^\dagger\rangle \\ \langle a_1 a_1^\dagger a_2\rangle & \langle a_1 a_1^\dagger a_2^\dagger a_2\rangle & \langle a_1^\dagger a_2\rangle & \langle a_1^\dagger a_2^\dagger a_2\rangle \\ \langle a_1 a_2 a_2^\dagger\rangle & \langle a_2^\dagger a_1\rangle & \langle a_1^\dagger a_1 a_2 a_2^\dagger\rangle & \langle a_1^\dagger a_2^\dagger a_1\rangle \\ \langle a_2 a_1\rangle & \langle a_1 a_2^\dagger a_2\rangle & \langle a_1^\dagger a_2 a_1\rangle & \langle a_1^\dagger a_1 a_2^\dagger a_2\rangle \end{pmatrix} \qquad (4)$$

which is constructed with the help of the conventional set of multiindices $\mathcal{J} = \{(0,0); (0,1); (1,0); (1,1)\}$. The reduced (partial) density matrices of the first and the second mode read

$$\begin{pmatrix} \langle a_1 a_1^\dagger\rangle & \langle a_1^\dagger\rangle \\ \langle a_1\rangle & \langle a_1^\dagger a_1\rangle \end{pmatrix} \text{ and } \begin{pmatrix} \langle a_2 a_2^\dagger\rangle & \langle a_2^\dagger\rangle \\ \langle a_2\rangle & \langle a_2^\dagger a_2\rangle \end{pmatrix}, \qquad (5)$$

respectively. Note that both matrices (5) cannot be simultaneously obtained from the total density matrix (4) by conventional partial trace methods. This is a peculiar property of fermionic states which differs them from the bosonic ones.

Spectra of reduced states

To anticipate general results, let us begin with the simplest case of two fermionic modes that can be occupied by a system with a varying number of quasiparticles in a pure state $|\psi\rangle = c_{00}|00\rangle + c_{01}|01\rangle + c_{10}|10\rangle + c_{11}|11\rangle$. According to Example the total density matrix (4) for such a state is $(c_{00}, c_{01}, c_{10}, c_{11})^\top (\overline{c_{00}}, \overline{c_{01}}, \overline{c_{10}}, \overline{c_{11}})$ and corresponds to the pure state indeed, whereas the reduced density matrices (5) take the form

$$\Lambda_1 = \begin{pmatrix} |c_{00}|^2 + |c_{01}|^2 & c_{00}\overline{c_{10}} + c_{01}\overline{c_{11}} \\ \overline{c_{00}}c_{10} + \overline{c_{01}}c_{11} & |c_{10}|^2 + |c_{11}|^2 \end{pmatrix},$$

$$\Lambda_2 = \begin{pmatrix} |c_{00}|^2 + |c_{10}|^2 & c_{00}\overline{c_{01}} - c_{10}\overline{c_{11}} \\ \overline{c_{00}}c_{01} - \overline{c_{10}}c_{11} & |c_{01}|^2 + |c_{11}|^2 \end{pmatrix},$$

respectively. The spectra of Λ_1 and Λ_2 would be identical if and only if $\mathrm{Tr}(\Lambda_1) = \mathrm{Tr}(\Lambda_2)$ and $\mathrm{Tr}(\Lambda_1^2) = \mathrm{Tr}(\Lambda_2^2)$. The first condition always holds true whereas the second one reduces to $\mathrm{Tr}(\Lambda_1^2 - \Lambda_2^2) = 8\mathrm{Re}(c_{00}c_{11}\overline{c_{01}c_{10}}) = 0$.

Proposition 3 *The two-mode fermionic state $|\psi\rangle = c_{00}|00\rangle + c_{01}|01\rangle + c_{10}|10\rangle + c_{11}|11\rangle$ has equispectral reduced density operators if and only if* $\mathrm{Re}(c_{00}c_{11}\overline{c_{01}c_{10}}) = 0$.

Example 1 *Suppose $|\psi\rangle = \frac{1}{2}(|00\rangle + |01\rangle + |10\rangle + |11\rangle)$, then* $\mathrm{Spect}(\omega_1) = \{0, 1\}$ *whereas* $\mathrm{Spect}(\omega_2) = \{\frac{1}{2}, \frac{1}{2}\}$.

Theorem 1 *Suppose that a pure state ω satisfies the parity superselection rule. Then, the spectra of ω_1 and ω_2 coincide.*

Theorem 2 *Suppose that for a pure state $|\psi\rangle\langle\psi|$ the partial states ω_1 and ω_2 have identical spectra. Then, there exist a state $|\phi\rangle\langle\phi|$ satisfying the parity superselection rule and unitary operators $U_1 \in \mathcal{A}_1$, $U_2 \in \mathcal{A}_2$ such that the partial states of $|U_2 U_1 \phi\rangle\langle U_2 U_1 \phi|$ coincide with ω_i, $i = 1, 2$. If the spectra of ω_i are simple (nondegenerate), then $|\psi\rangle = U_1 U_2 |\phi\rangle$.*

Conclusions

We have fully characterized general pure fermionic states such that their reduced density matrices are equispectral. Equispectrality automatically takes place for bosonic systems and systems of distinguishable particles, however, it does not necessarily holds true for systems composed of indistinguishable fermionic quasiparticles. On the other hand, equispectrality is a natural quantum information property that reflects the fact that entropies of subsystems must coincide. We have found necessary and sufficient conditions for spectra of partial states to be identical. As a byproduct of our research, we have analyzed the density matrix formalism for general case of fermionic states and provided the explicit construction of density matrices (Corollary 2 and Example). The developed formalism clearly indicates that the conventional partial trace methods are not applicable to fermionic states.

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